



Jet Propulsion Laboratory
California Institute of Technology

Optimal Estimation for Imaging Spectrometer Atmospheric Correction

Remote Sensing of Environment 216 (2018), 355-373.

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Optimal estimation for imaging spectrometer atmospheric correction

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² NASA Goddard Space Flight Center

³ Naval Research Laboratory

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**The open source code is
available through the open
source ISOFIT project:**

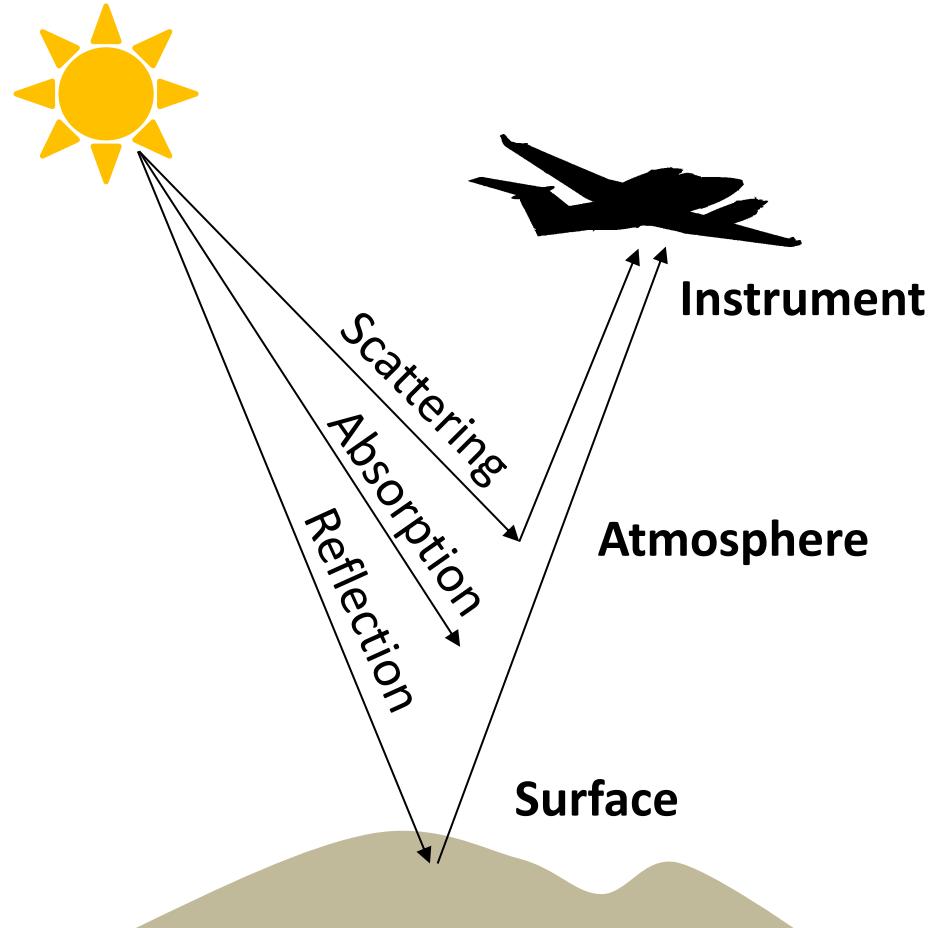
<https://github.com/isofit/isofit>

Contact us if you'd like to contribute.

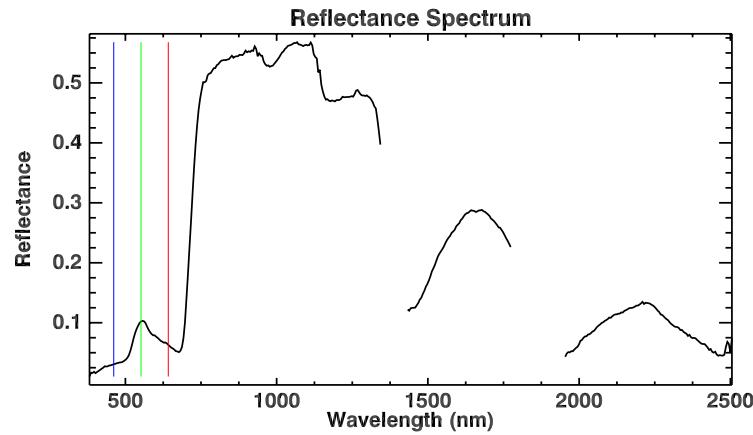
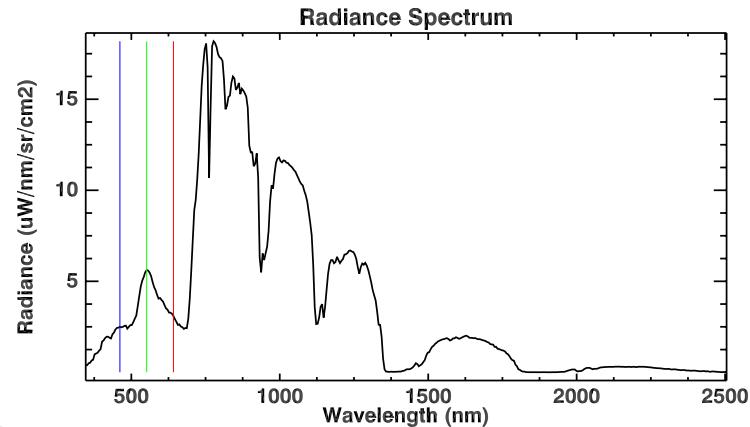
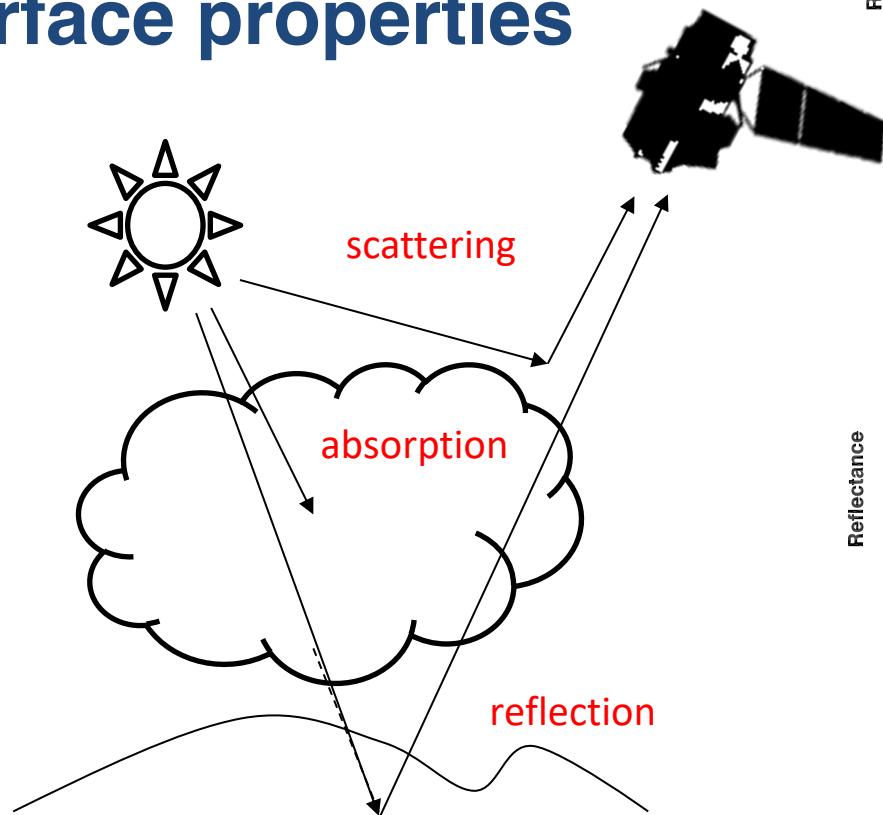


Agenda

1. Motivation
2. Mathematical foundations
3. Field experiments
4. Operational considerations, future steps



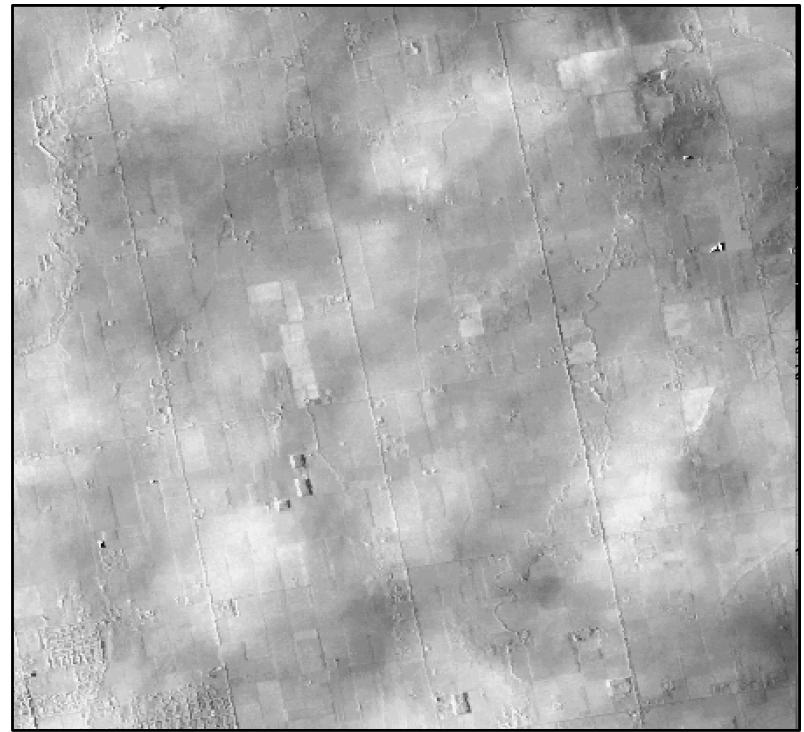
Visible/Shortwave IR spectra are sensitive to both atmosphere & surface properties



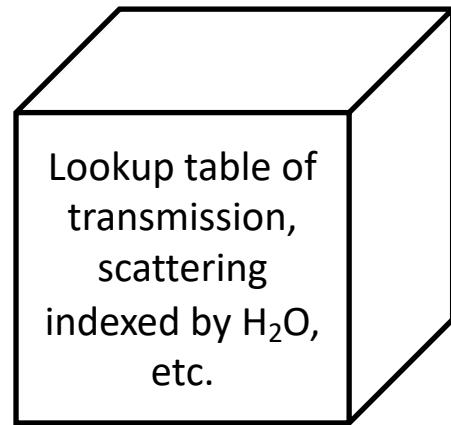
Atmosphere varies over short spatiotemporal scales

“AVIRIS Classic” imaging spectrometer, visible wavelengths

Retrieved Water vapor
[Thompson et al., *Surv. Geohysics*, 2018]



Conventional atmospheric correction: A sequential process



- 1. In advance, do RTM calculations**

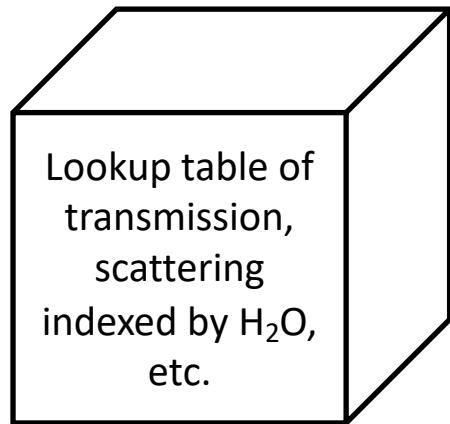
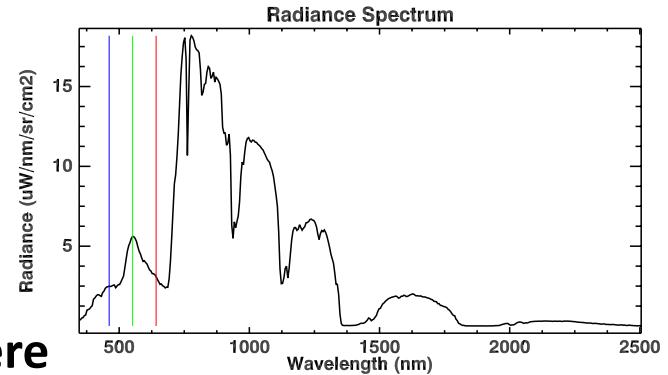


david.r.thompson@jpl.nasa.gov

5 March 2018

Conventional atmospheric correction: A sequential process

2. Estimate atmosphere
(typically by band ratios)



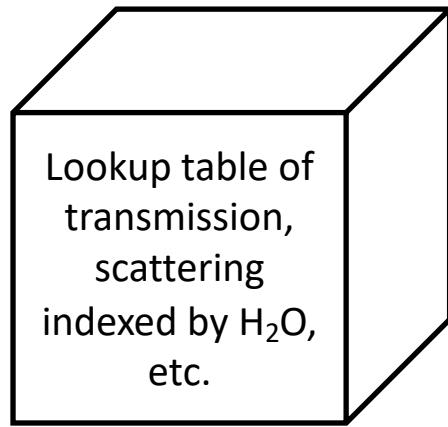
1. In advance, do RTM calculations



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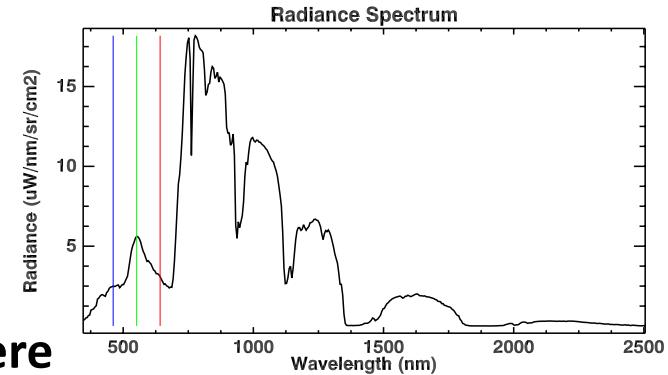
5 March 2018

Conventional atmospheric correction: A sequential process



1. In advance, do
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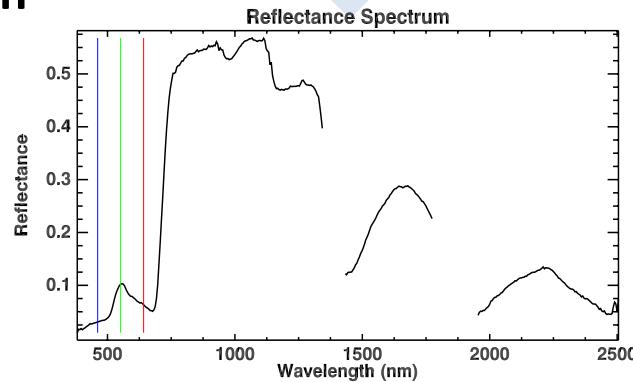


reflectance

measurement

$$\rho_{obs}^* = \rho_a + \frac{T\rho_s}{1 - S\rho_s}$$

3. Algebraic
Inversion



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5 March 2018



Limitations of conventional methods

1. Limited size of state vector that can be represented in the lookup table
2. Algebraic approximate solutions are less accurate for extreme geometries
3. Do not couple surface and atmosphere
4. Estimate atmosphere independently, making it difficult to disambiguate smooth atmospheric effects from surface effects
5. Disregard uncertainties



Global spectroscopy missions are an atmospheric correction challenge

Sequential methods face difficulties in certain observing conditions:

- High water vapor
- Extreme viewing angles
- Surface/atmosphere coupling
- Heavy aerosol loads

Orbital missions access tropical and subtropical environments that:

- Host a large fraction of Earth's productivity and biodiversity
- Are underrepresented in atmospheric correction research
- Often have “difficult” atmospheres



Optimal Estimation Theory: Simultaneous estimation of surface and atmosphere

- **A true spectroscopic retrieval** that can exploit information distributed across the spectrum, helping to disentangle surface and atmosphere
- **A rigorous probabilistic formulation** incorporates ancillary measurements via the prior distribution
- **Comprehensive uncertainty estimates** can inform downstream analyses and global maps
- **Flexible state vectors** that might be more robust for difficult observing conditions
- **Elegant, conceptually simple 1-step estimation**



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AVIRIS-NG Installation

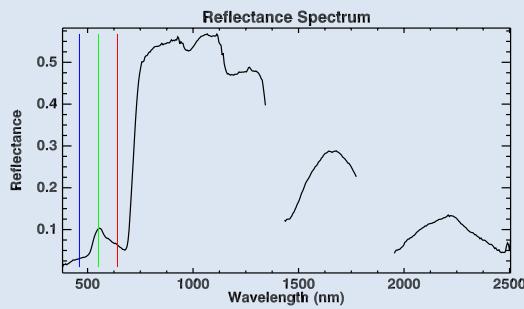


The “forward problem”

State vector

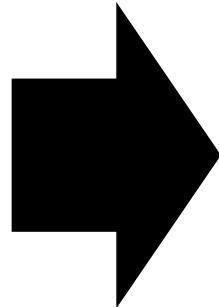
$$\mathbf{x} \in \mathbb{R}^N$$

$$\mathbf{x} = \begin{bmatrix} \text{Surface parameters} \\ \dots \\ \text{Atmosphere parameters} \\ \dots \\ \text{Instrument parameters} \\ \dots \end{bmatrix}$$



Forward model

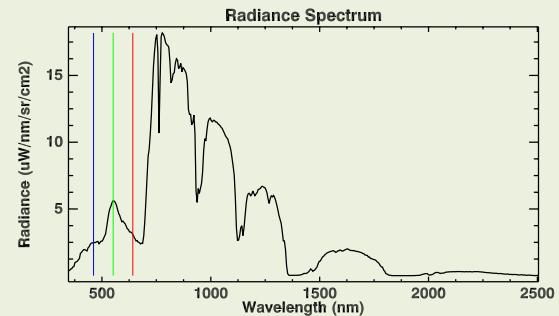
$$F(\mathbf{x}) : \mathbb{R}^N \mapsto \mathbb{R}^M$$



Measurement

$$\mathbf{y} \in \mathbb{R}^M$$

$$\mathbf{y} = \begin{bmatrix} \text{Calibrated at-aperture} \\ \text{radiance measurements} \end{bmatrix}$$

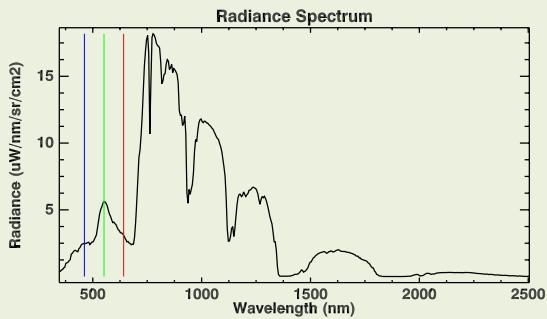


The “inverse problem”

Measurement

$$\mathbf{y} \in \mathbb{R}^M$$

$$\mathbf{y} = \begin{bmatrix} \text{Calibrated at-aperture} \\ \text{radiance measurements} \end{bmatrix}$$



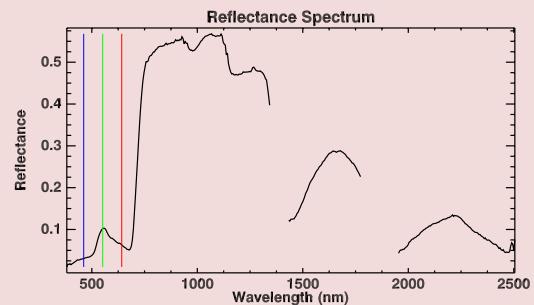
Inversion algorithm

$$R(\mathbf{y}) : \mathbb{R}^M \mapsto \mathbb{R}^N$$

Estimated state vector

$$\hat{\mathbf{x}} \in \mathbb{R}^N$$

$$\hat{\mathbf{x}} = \begin{bmatrix} \text{Estimated surface parameters} \\ \dots \\ \text{Estimated atmosphere parameters} \\ \dots \\ \text{Estimated instrument parameters} \\ \dots \end{bmatrix}$$



Maximum *A Posteriori* solution

$$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{p(\mathbf{y})}$$



Maximum *A Posteriori* solution

$$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{p(\mathbf{y})}$$

The *Maximum A Posteriori* estimation is equivalent to the optimization:

$$\chi^2(\mathbf{x}) = (\mathbf{F}(\mathbf{x}) - \mathbf{y})^T \mathbf{S}_\epsilon^{-1} (\mathbf{F}(\mathbf{x}) - \mathbf{y}) + (\mathbf{x} - \mathbf{x}_a)^T \mathbf{S}_a^{-1} (\mathbf{x} - \mathbf{x}_a)$$

Cost

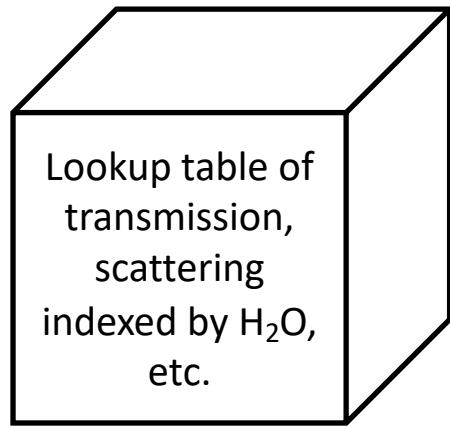
Model match to measurement

Bayesian prior

... we can solve it by conjugate gradient descent.

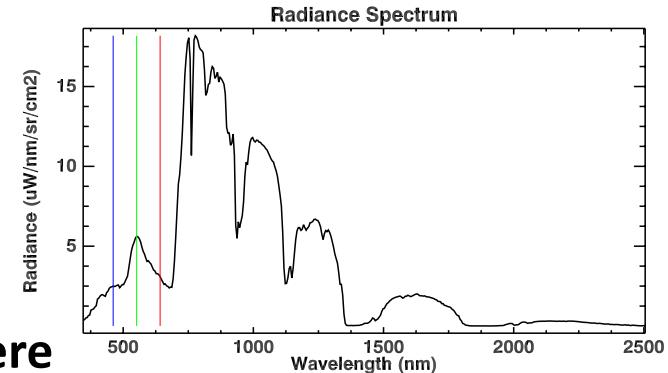


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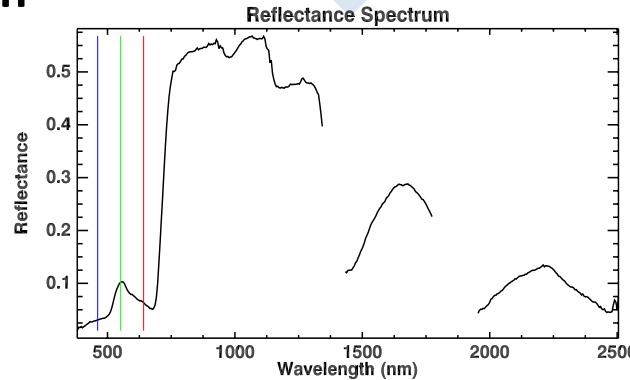


measurement

reflectance

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3. Algebraic
Inversion



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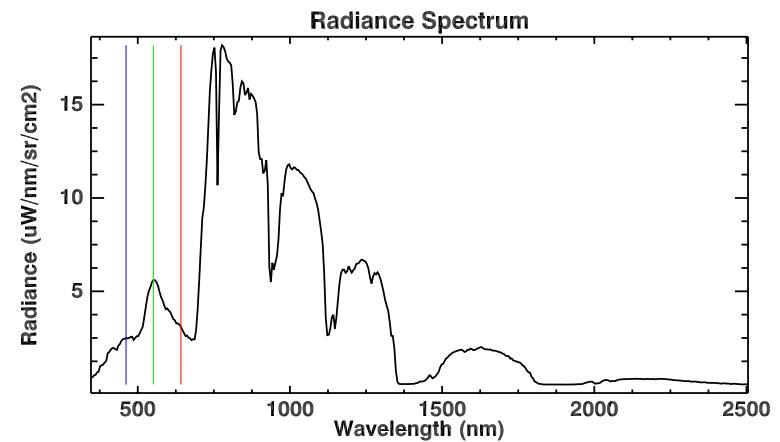
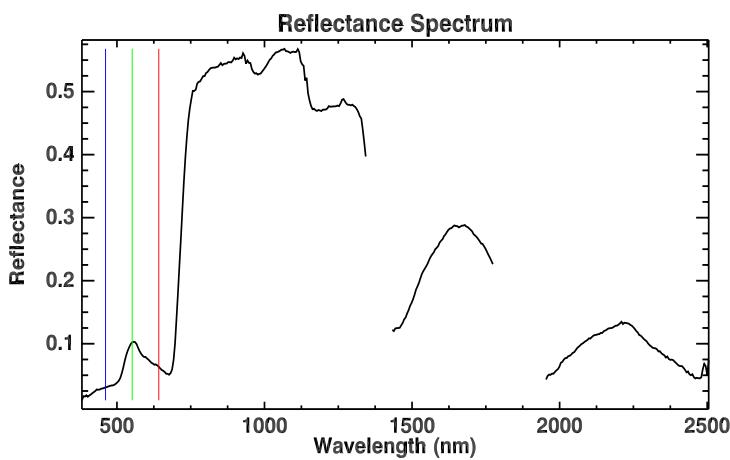
5 March 2018



Iterative simultaneous estimation of atmosphere and surface

1. Predict
radiance

$$y = F(x) + \epsilon$$



2. Optimize
state vector

$$\chi^2(x) = \underbrace{(F(x) - y)^T S_\epsilon^{-1} (F(x) - y)}_{\text{Cost}} + \underbrace{(x - x_a)^T S_a^{-1} (x - x_a)}_{\text{Model match to measurement}} + \underbrace{(x - x_a)^T S_a^{-1} (x - x_a)}_{\text{Bayesian prior}}$$



Variability due to measurement noise vs. unknown state parameters

Total observation noise

$$\mathbf{S}_\epsilon = \mathbf{S}_y + \mathbf{K}_b \mathbf{S}_b \mathbf{K}_b^T$$

Measurement noise
(instrument effects)

- Photon noise
- Read noise
- Dark current noise

Jacobian WRT unknowns

$$\mathbf{S}_\epsilon = \mathbf{S}_y + \mathbf{K}_b \mathbf{S}_b \mathbf{K}_b^T$$

Unknown parameters in the
observation system

- Sky view factor
- H₂O absorption coefficient intensity
- Systematic radiative transfer error
- Uncorrelated radiative transfer error



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AVIRIS-NG Installation



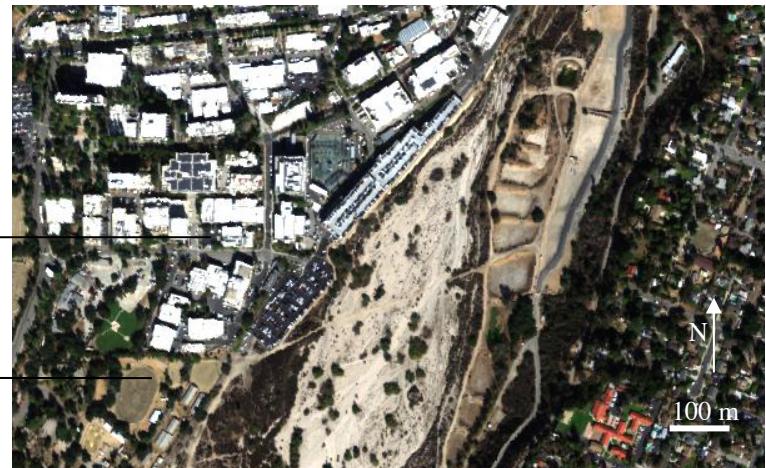
Case study

- Sites visited by Mark Helmlinger, Scott Nolte
- In-situ AOD via Reagan sunphotometers
- In-situ surface reflectance via ASD FieldSpec

Ivanpah Playa



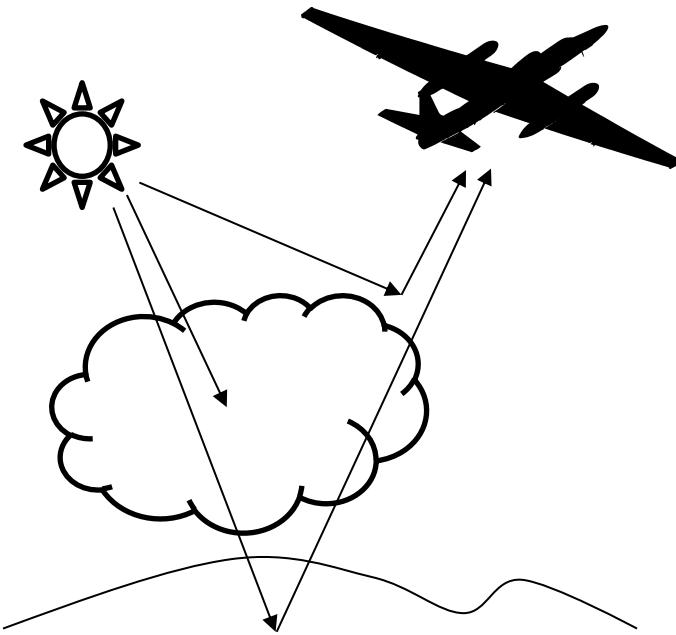
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From Thompson et al., RSE (in review)



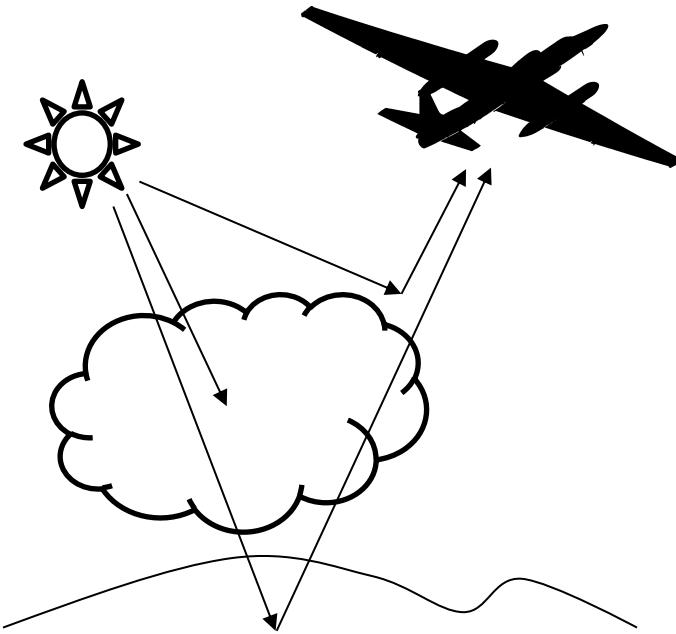
Instrument: AVIRIS-NG

Atmosphere: MODTRAN 6.0 RTM

Model components

Surface: Multi-component Multivariate
Gaussians





Model components

Pre-defined

Instrument: AVIRIS-NG

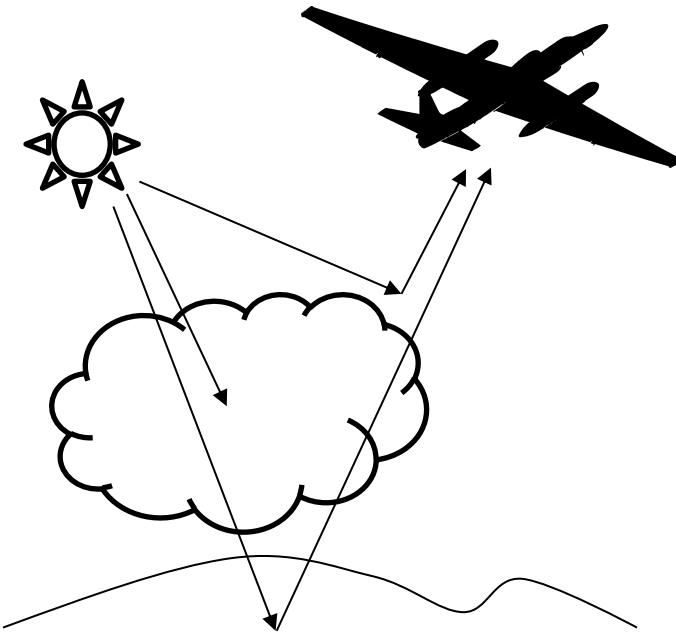
- Instrument model with Wavelength- and signal-dependent SNR
- Photon shot & read noise

Atmosphere: MODTRAN 6.0 RTM

- DISORT MS, Correlated-k
- Rural aerosol model

Surface: Multi-component Multivariate Gaussians





Model components

Pre-defined
Statistical, fit to data

Instrument: AVIRIS-NG

- Instrument model with Wavelength- and signal-dependent SNR
- Photon shot & read noise
- Uncorrelated calibration uncertainty
- Systematic calibration / RT uncertainty

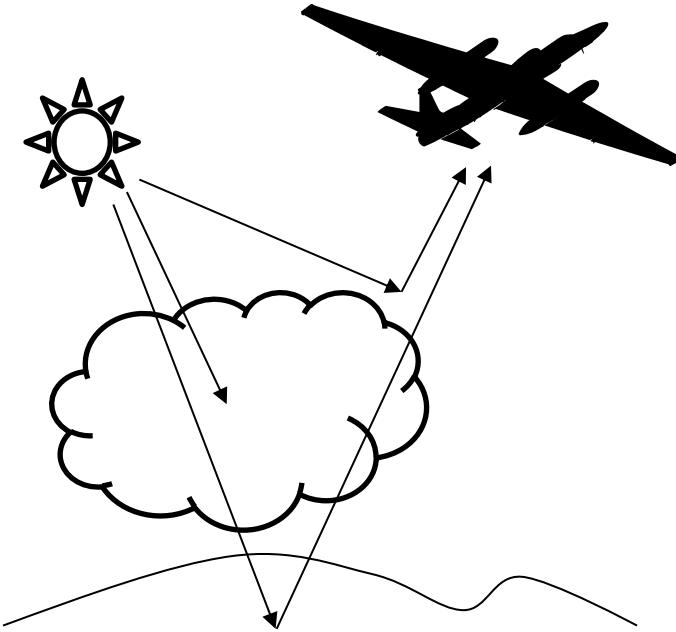
Atmosphere: MODTRAN 6.0 RTM

- DISORT MS, Correlated-k
- Rural aerosol model
- broad prior uncertainties
- Unmodeled unknowns, including H_2O absorption coefficients

Surface: Multi-component Multivariate Gaussians

- Prior based on universal library, highly regularized to permit accurate retrieval of arbitrary shapes





Model components

Pre-defined
Statistical, fit to data
Retrieved in the inversion

Instrument: AVIRIS-NG

- Instrument model with Wavelength- and signal-dependent SNR
- Photon shot & read noise
- Uncorrelated calibration uncertainty
- Systematic calibration / RT uncertainty

Atmosphere: MODTRAN 6.0 RTM

- DISORT MS, Correlated-k
- Rural aerosol model
- broad prior uncertainties
- Unmodeled unknowns, including H_2O absorption coefficients
- H_2O , AOD retrieved

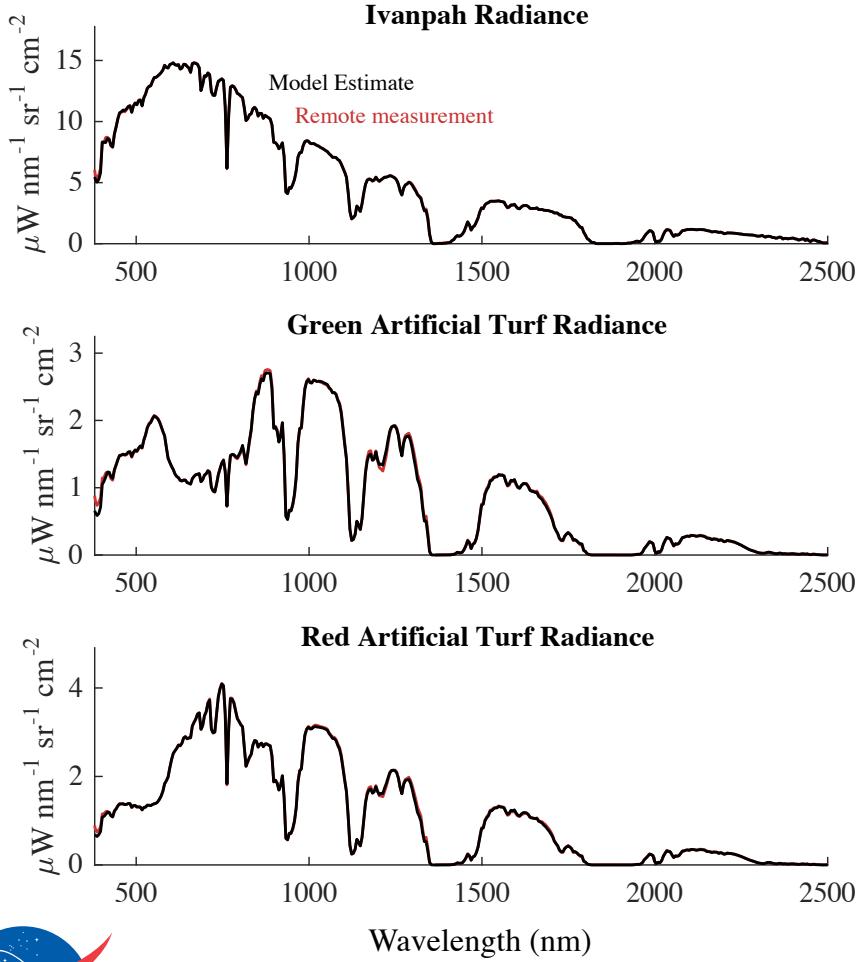
Surface: Multi-component Multivariate Gaussians

- Prior based on universal library, highly regularized to permit accurate retrieval of arbitrary shapes
- Reflectance estimated independently in every channel



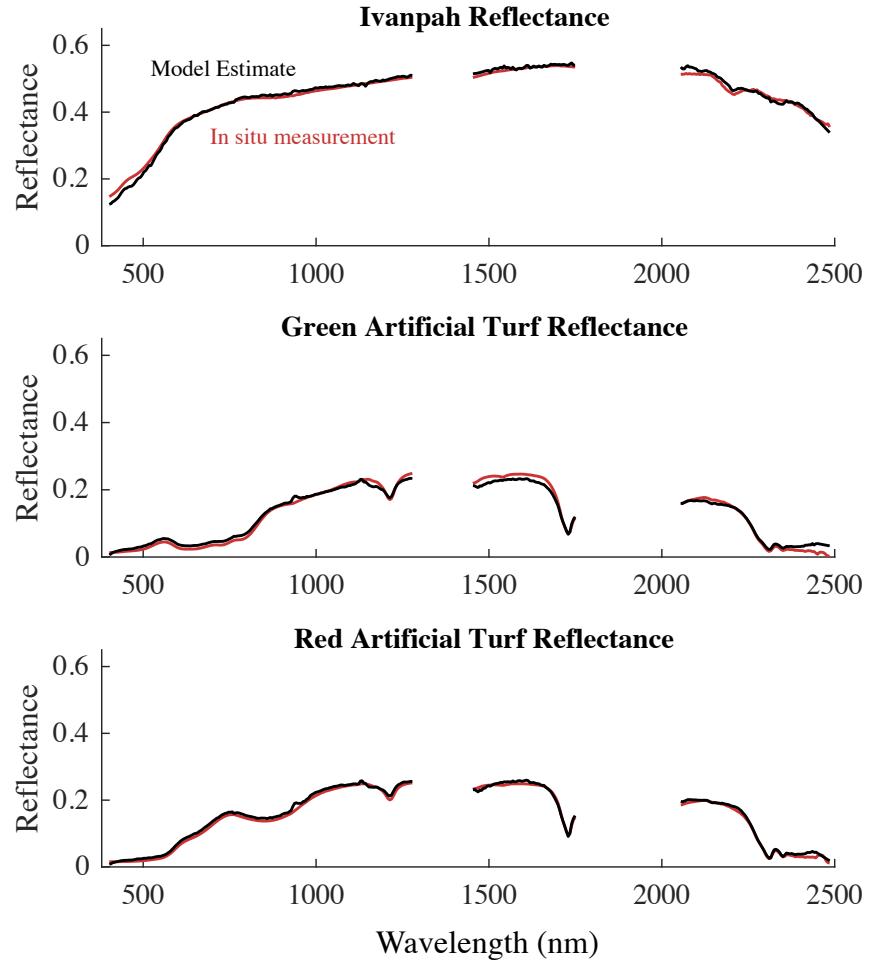
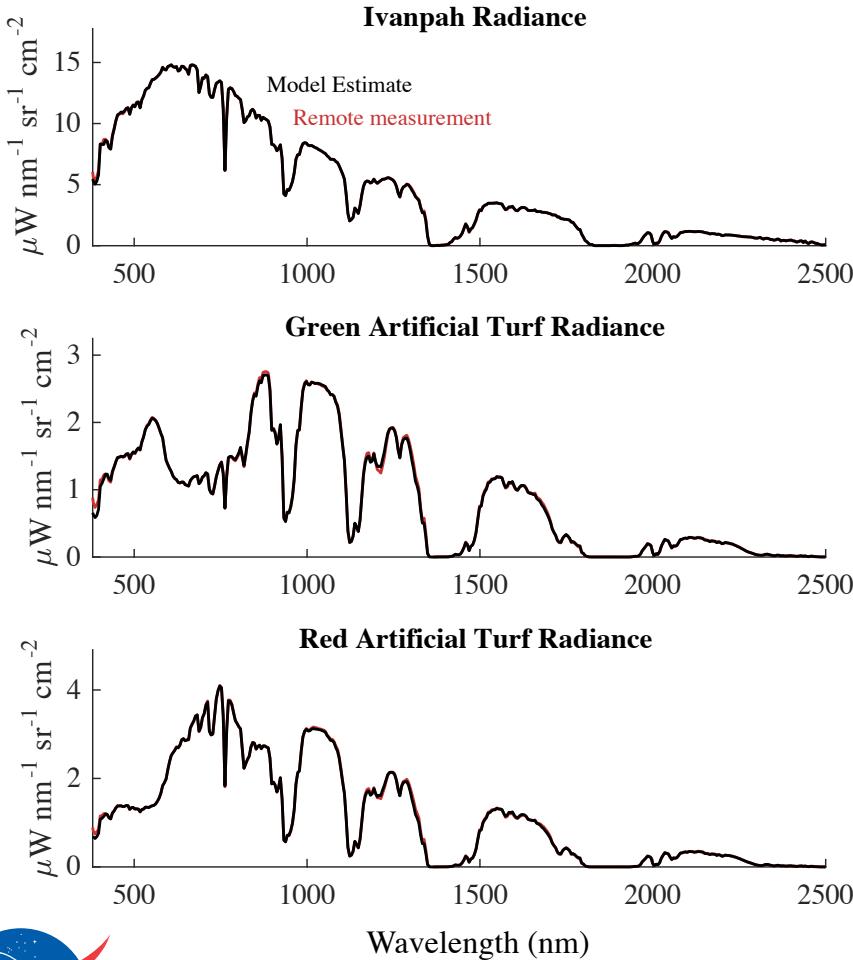
Radiance model vs. measurement

[Thompson et al., *Remote Sensing of Environment* 2018]



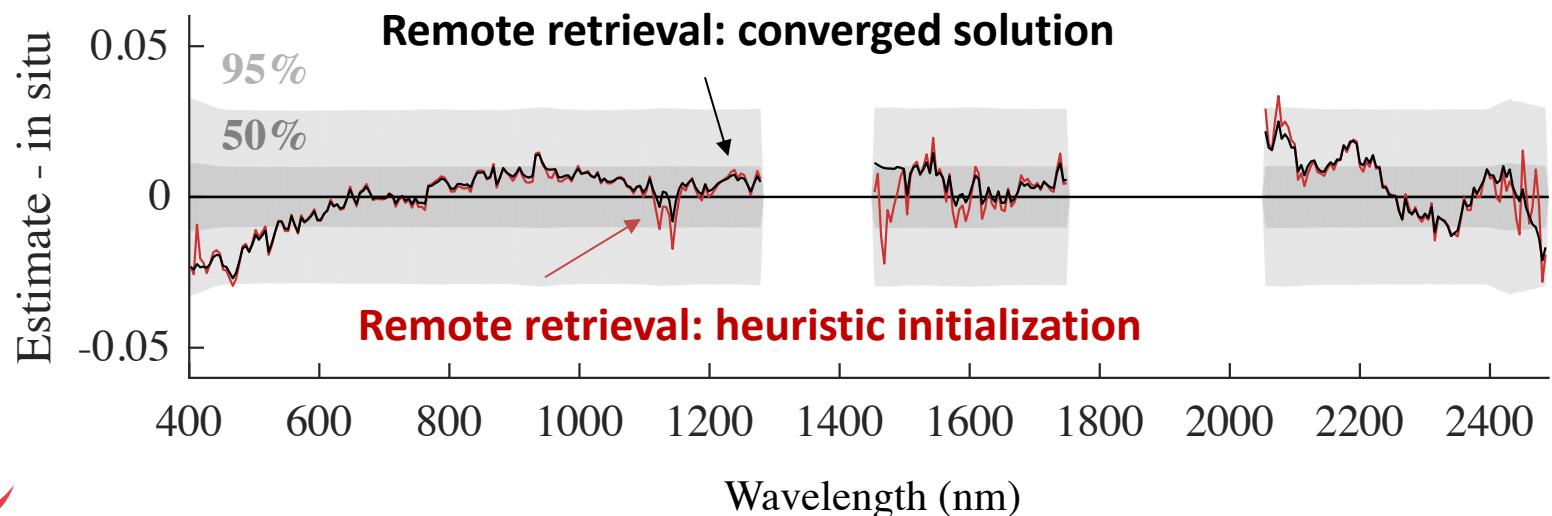
Reflectance estimate vs. in situ

[Thompson et al., *Remote Sensing of Environment* 2018]



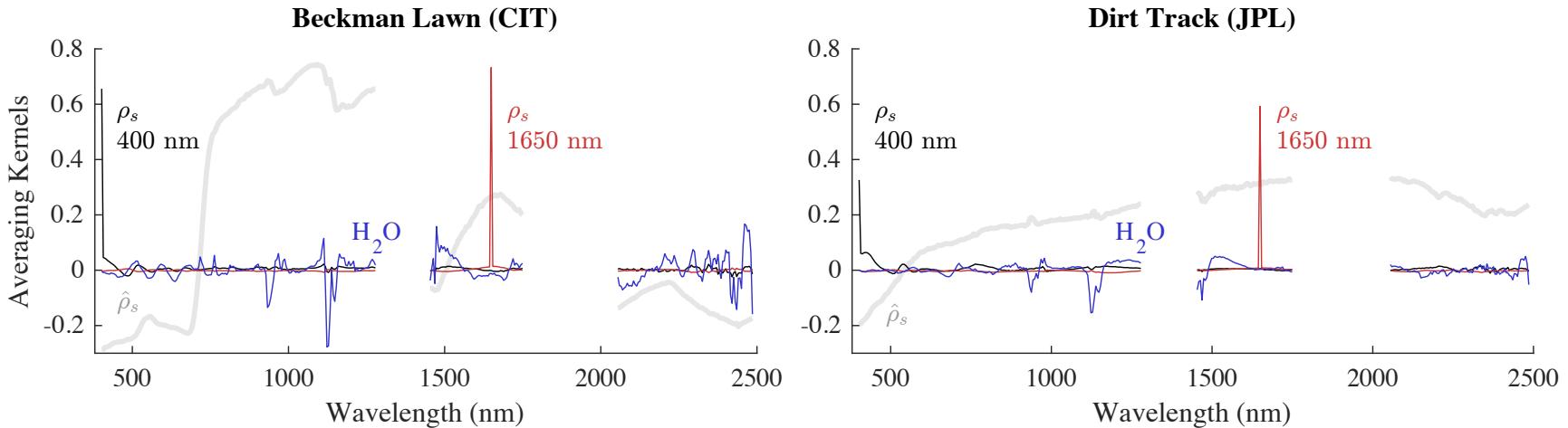
Posterior uncertainty compared to actual discrepancies

[Thompson et al., *Remote Sensing of Environment* 2018]



“Averaging Kernels”

Rows of the A matrix show sensitivity of the retrieval to different elements of the true state



E.G. The H₂O estimate transparently leverages information across the VSWIR spectrum (though mostly in the strong absorption features)



From Thompson et al., RSE (in review)

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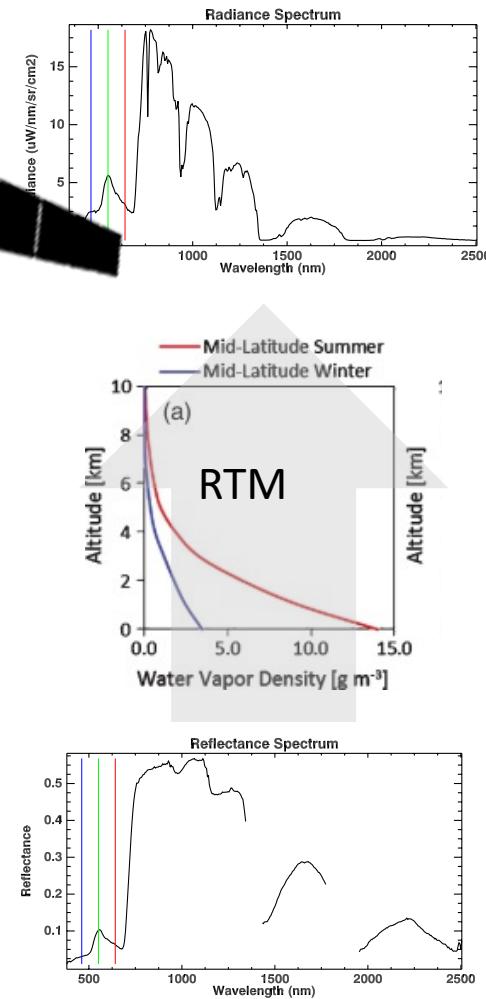
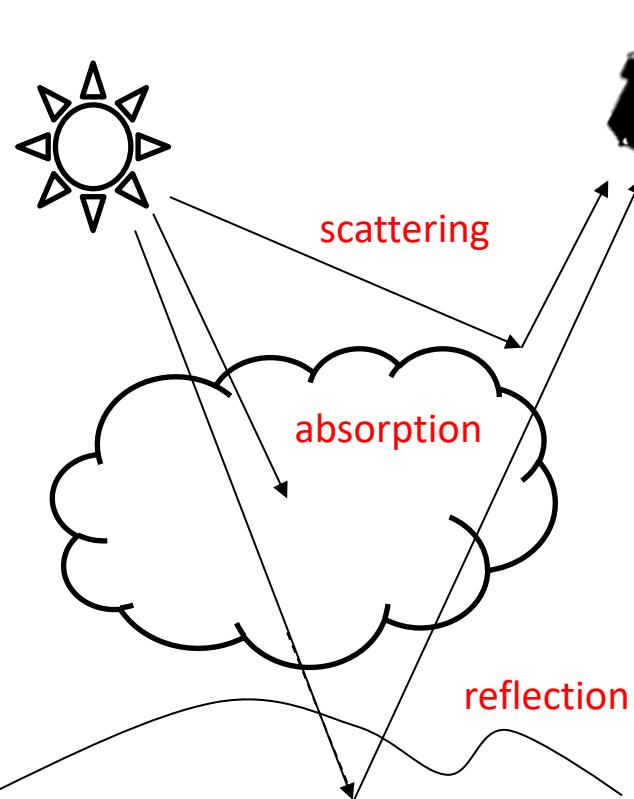


AVIRIS-NG Installation



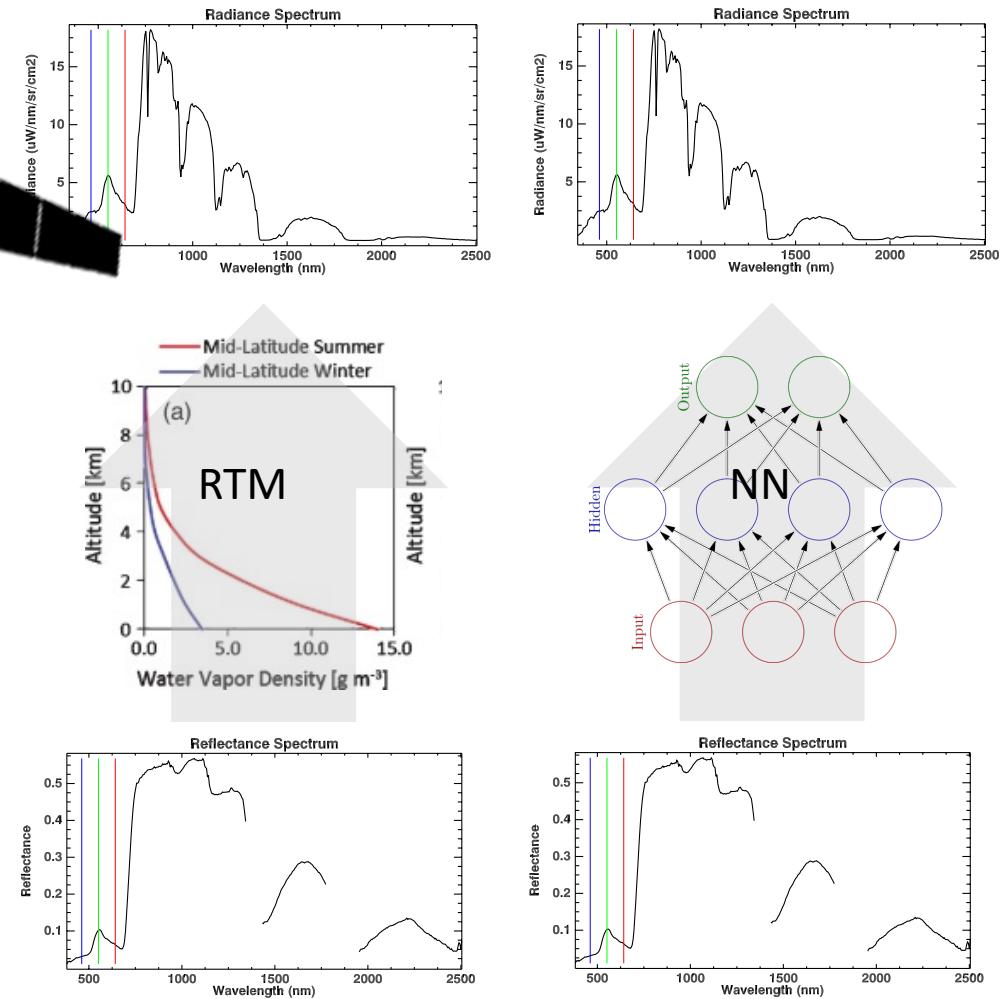
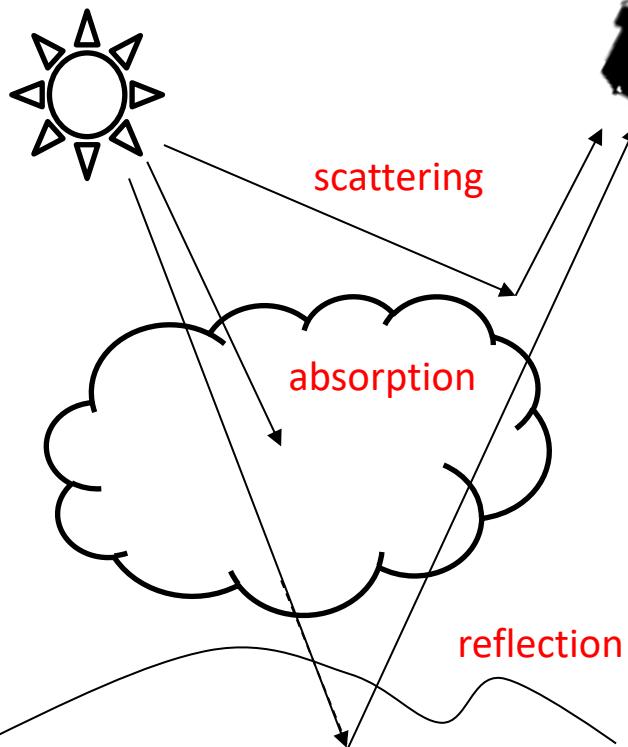
Speeding up the forward model

images: Mishra et al., Heliyon 2015, wikipedia



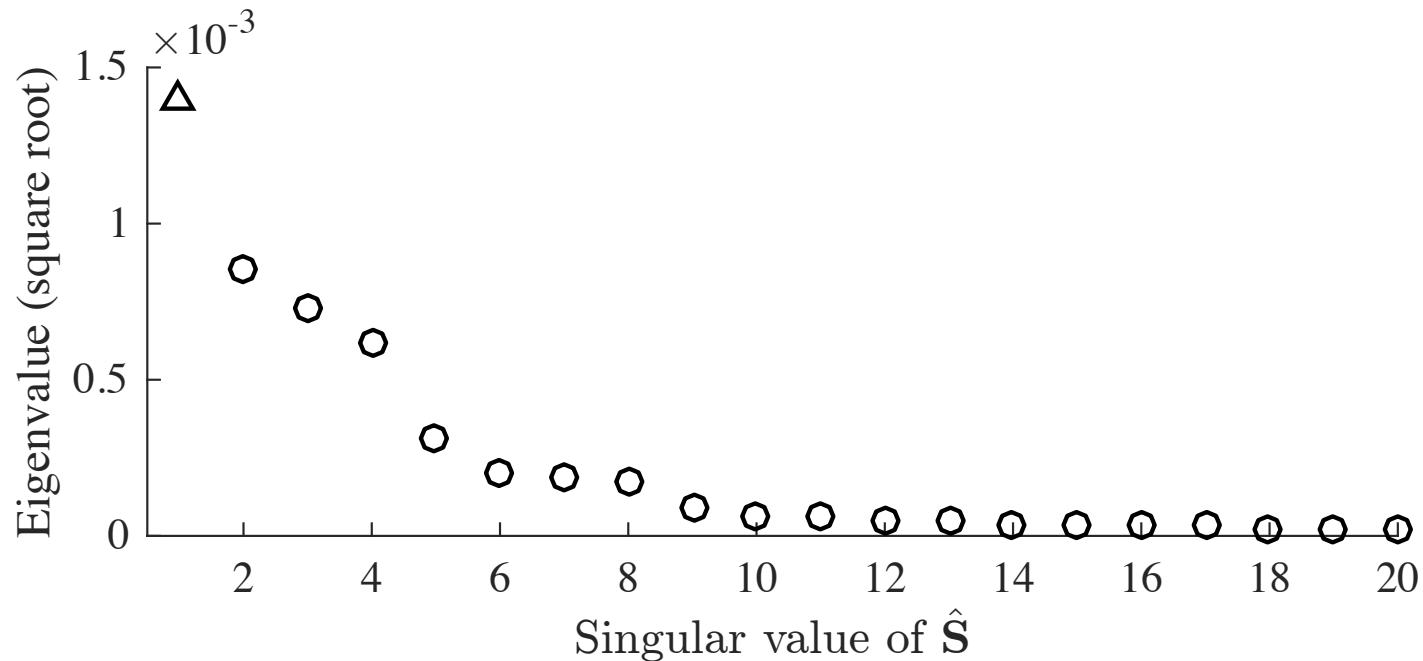
Speeding up the forward model

images: Mishra et al., Heliyon 2015, wikipedia



Operational Considerations: Data Volume of Uncertainties

It is not necessary to distribute the full error covariances for each spectrum— a few eigenvalues are enough.



Summary of optimal estimation

- A **true spectroscopic retrieval** that exploits information distributed across the spectrum, helping to disentangle surface and atmosphere
- A **rigorous probabilistic formulation** that incorporates ancillary measurements via the prior distribution
- A **general framework** that can incorporate many modeling choices and assumptions
- A **potential tool for global spectroscopy**



With due thanks to:

- **Kevin Bowman** (JPL), for much of the source material in these slides
- **Clive D. Rogers**, for theoretical foundations, approach and notation (e.g. *Inverse Methods for Atmospheric Sounding, Theory and Practice*, 2000).
- **NASA Earth Science** for sponsorship of AVIRIS-NG and the AVIRIS-NG India investigation and analysis.
- **The JPL Research and Technology Development and NASA Center Innovation Fund Programs**
- **The JPL Office of Chief Scientist and Technologist**
- **Other coinvestigators, coauthors and colleagues** including Amy Braverman, Jonathan Hobbs, Robert Spurr, Steven Massie, Bruce Kindel, Manoj Mishra, et cetera.





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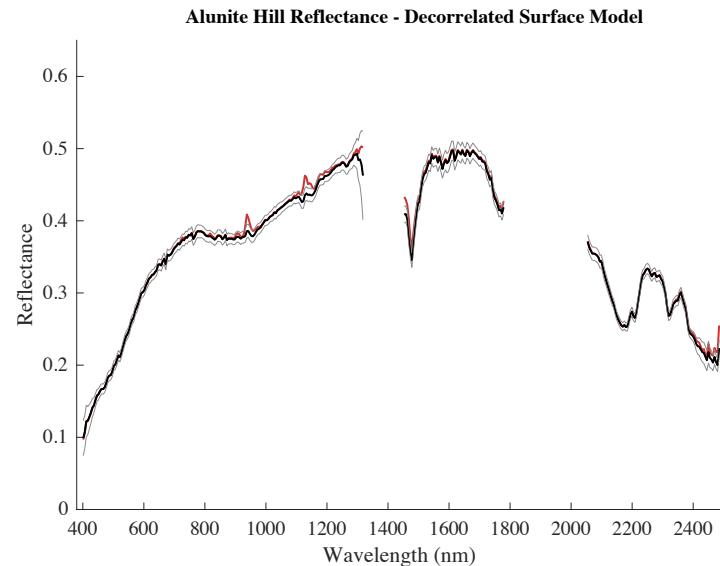
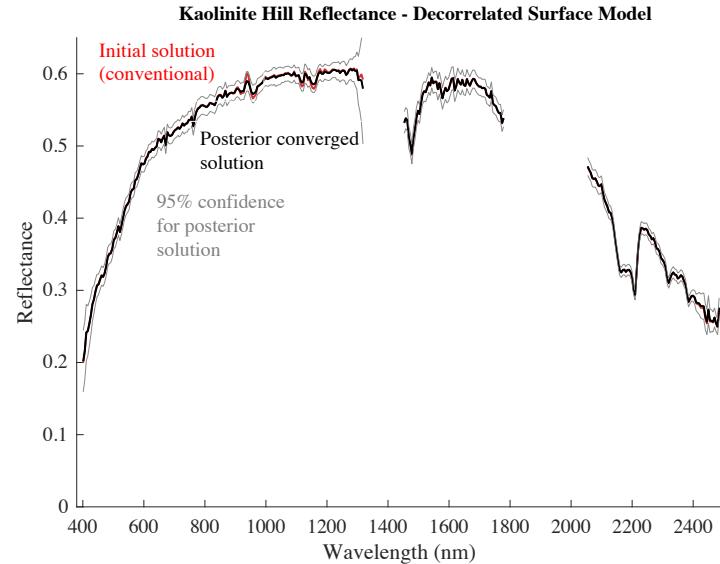
Backup slides

Operational Considerations: Smoothing error

General purpose products (i.e. for broad distribution) can use unconstrained surfaces, decorrelating wavelengths outside atmospheric intervals to:

- Preserve the numerical proportion between neighboring wavelengths, facilitating downstream calculation of gain corrections or PLSR coefficients
- Eliminate any chance of “missing” unanticipated features
- Preserve the ability to calculate uncertainties

Investigators could still use custom surface models for specific studies



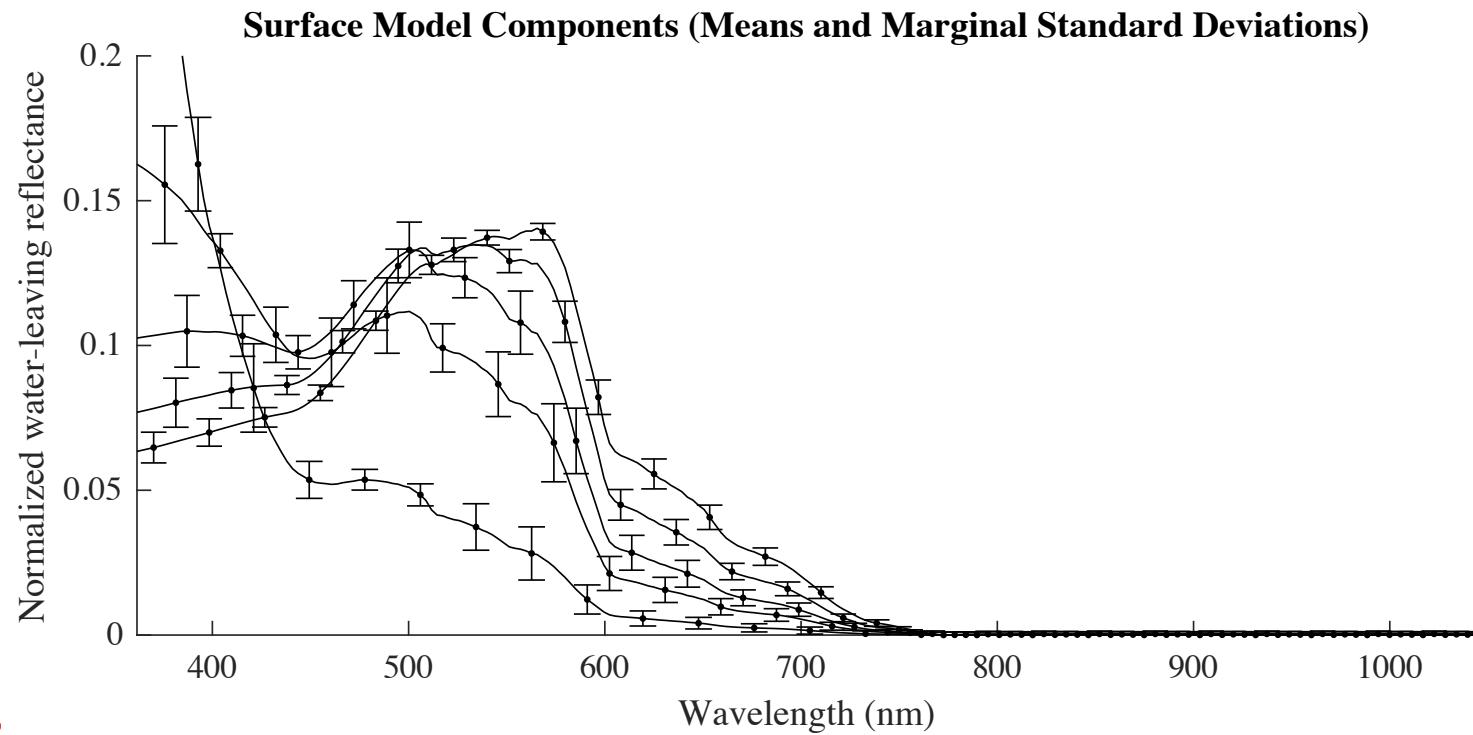
Application to Ocean Scenes

- PRISM instrument over Santa Monica Bay
- More constrained surface reflectance
- Improve cross-track uniformity with columnwise geometry and instrument-noise models

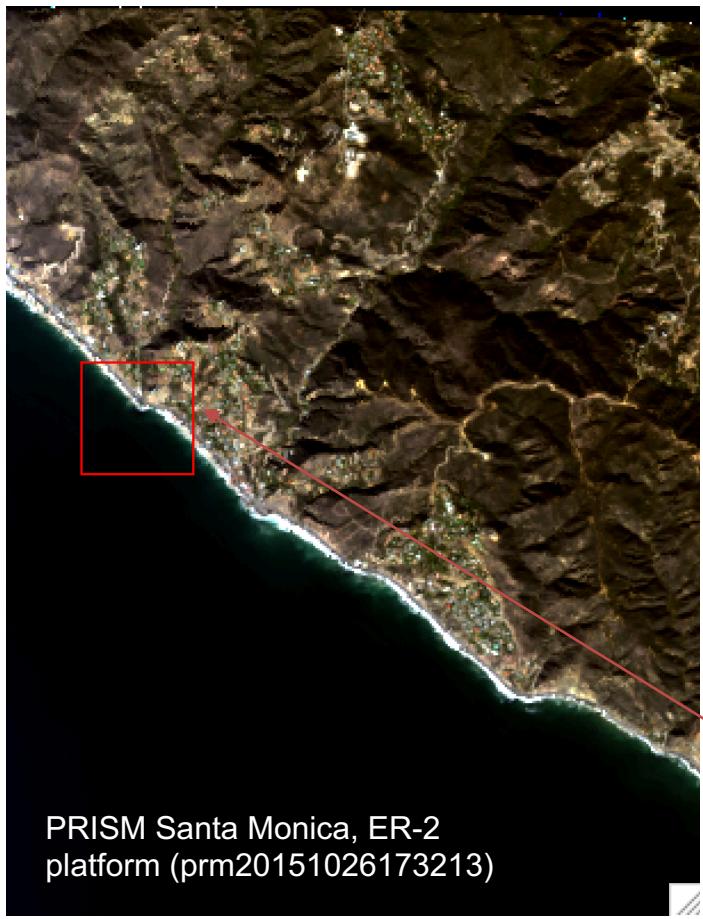


Application to Ocean Scenes

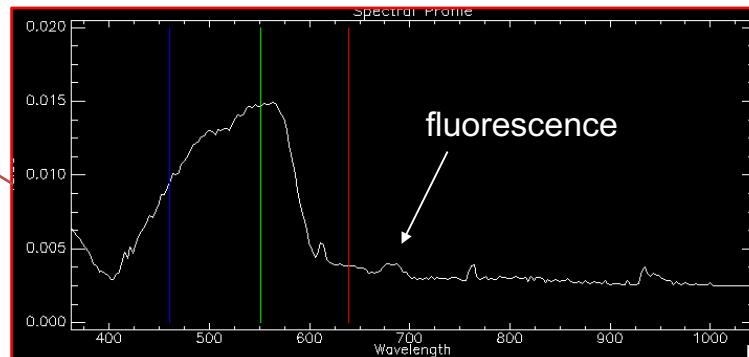
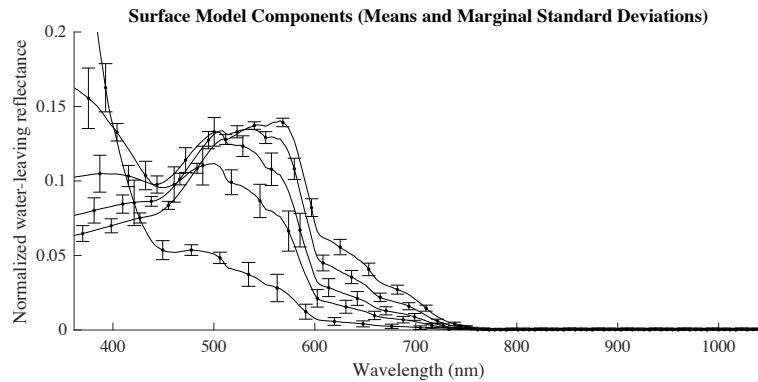
- Synthesize surface reflectances using a four-parameter model of water properties (Lee et al., 2004)



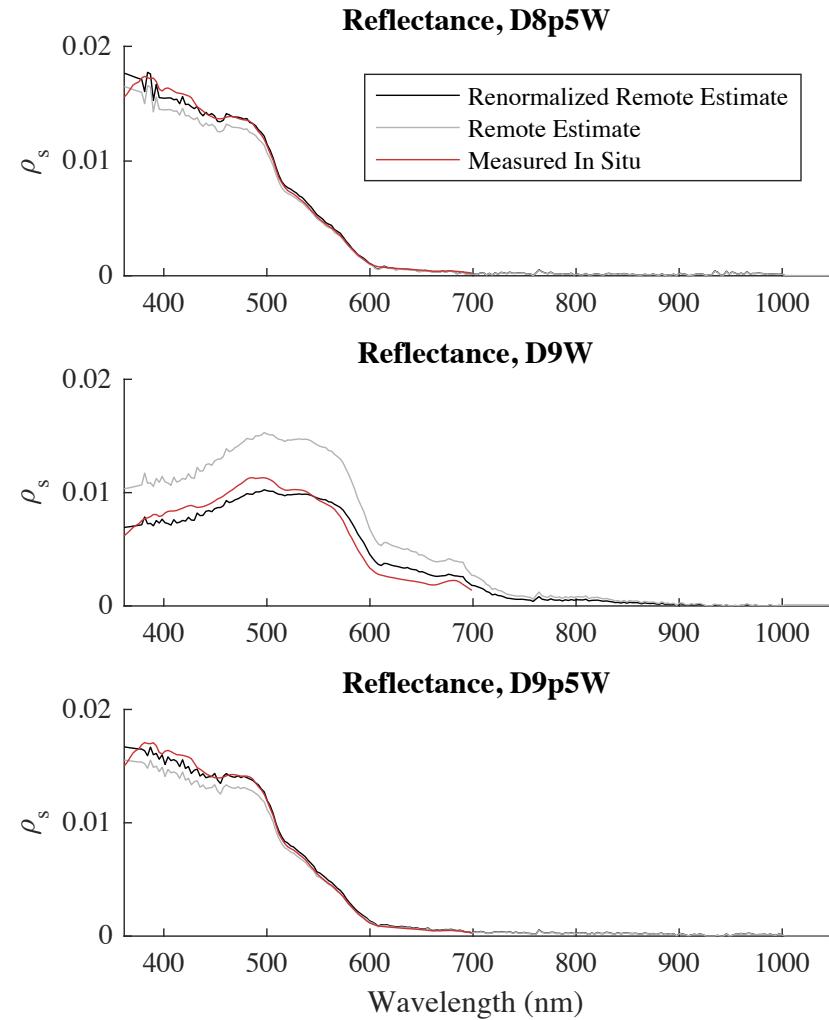
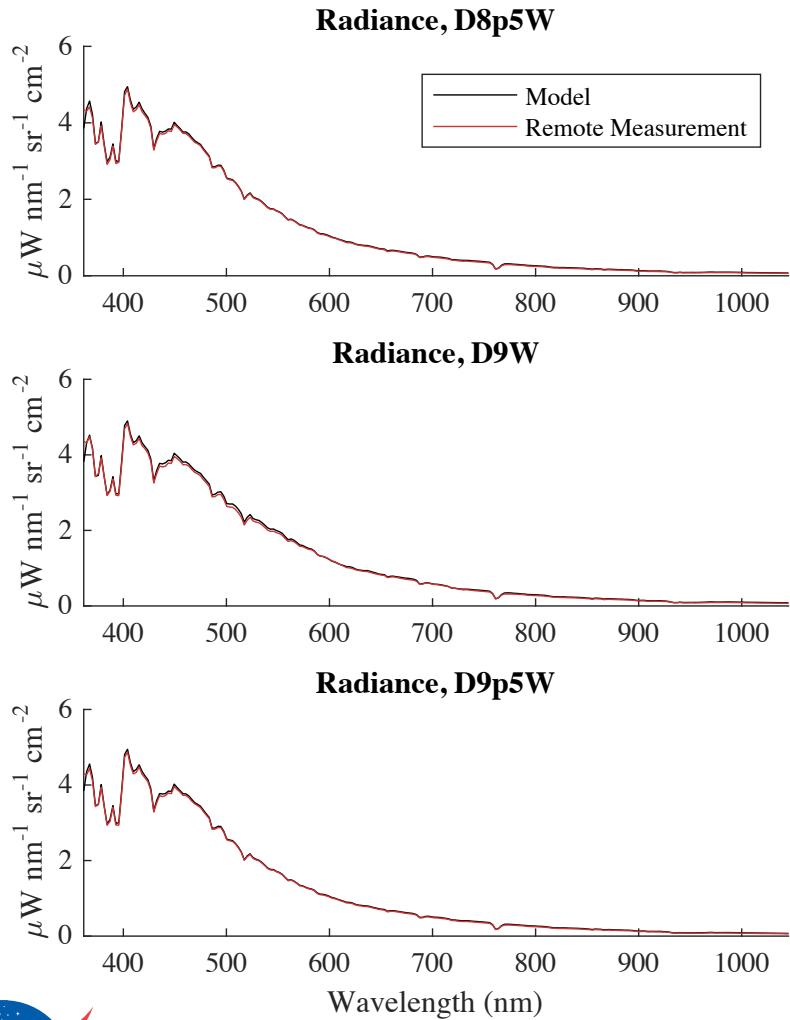
Application to Ocean Scenes



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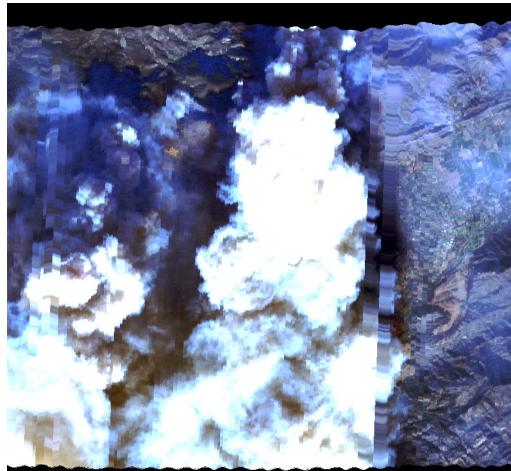
Application to Ocean Scenes



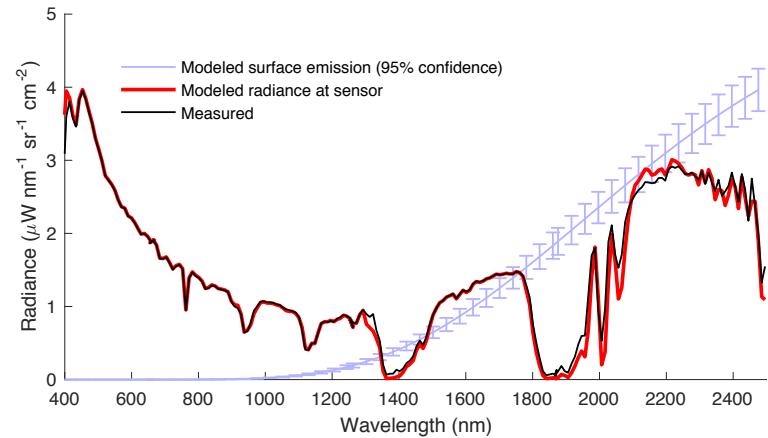
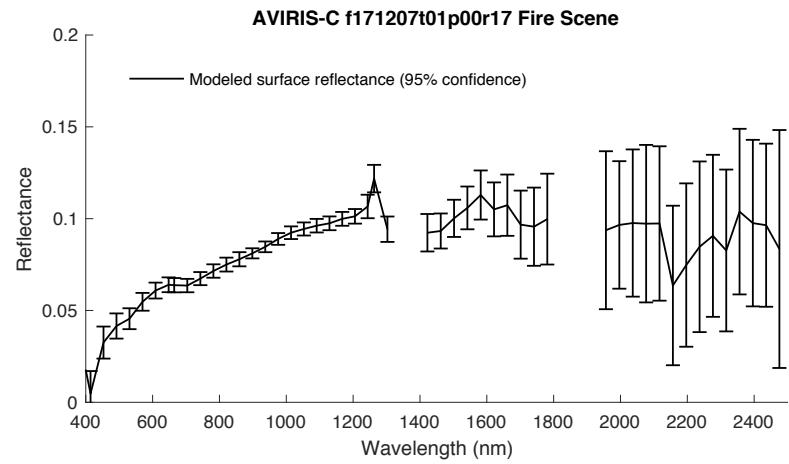
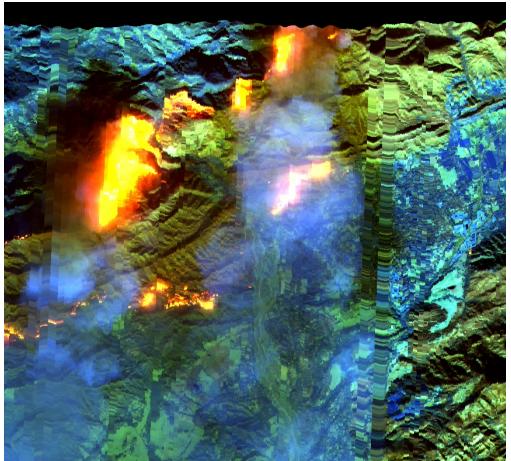
Application to Emissive surfaces

12/7/17,
During
Thomas
Fire

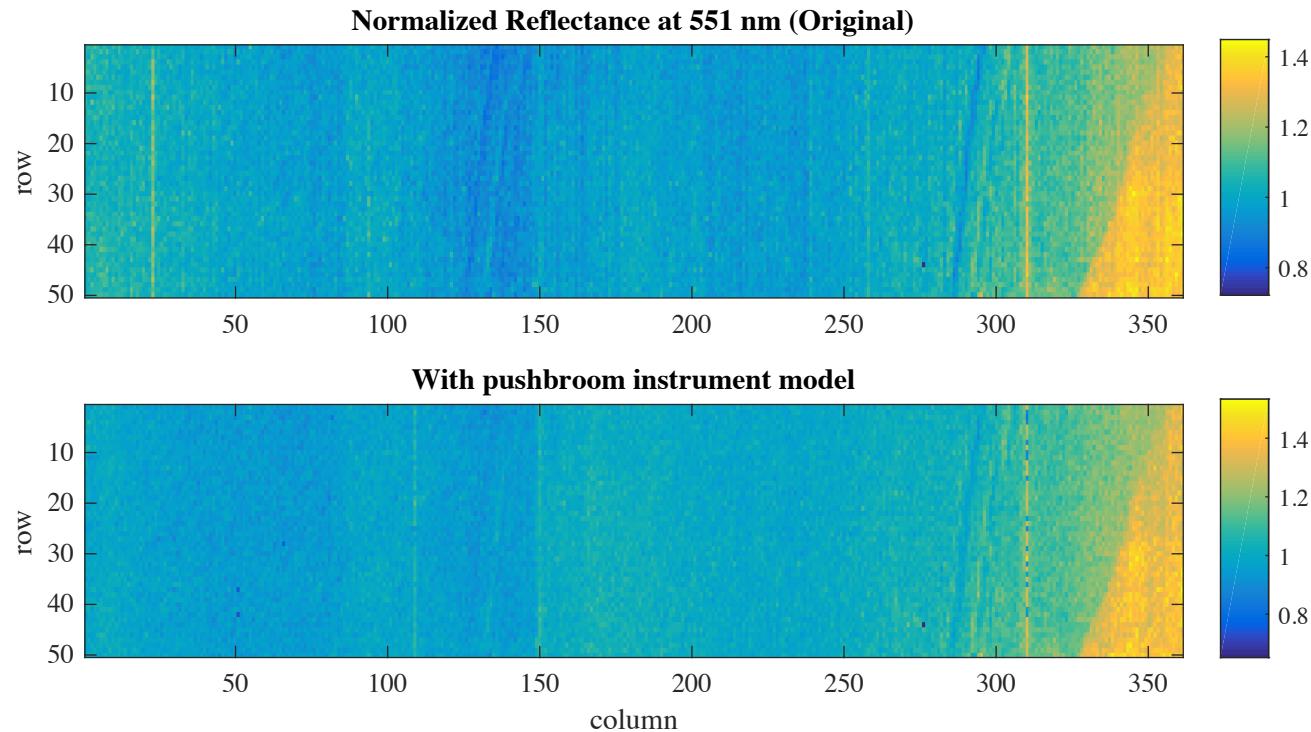
Visible
image
R: 650 nm
G: 550 nm
B: 450 nm)



Infrared
image
(R: 2250 nm
G: 1650 nm
B: 1000 nm)



Application to Ocean Scenes



Characterization

The Gain Matrix: retrieval sensitivity to a change in \mathbf{F}

$$\mathbf{G} = \frac{\partial \hat{\mathbf{x}}}{\partial \mathbf{F}} = (\mathbf{K}^\top \mathbf{S}_n^{-1} \mathbf{K} + \mathbf{S}_a^{-1})^{-1} \mathbf{K}^\top \mathbf{S}_n^{-1}$$

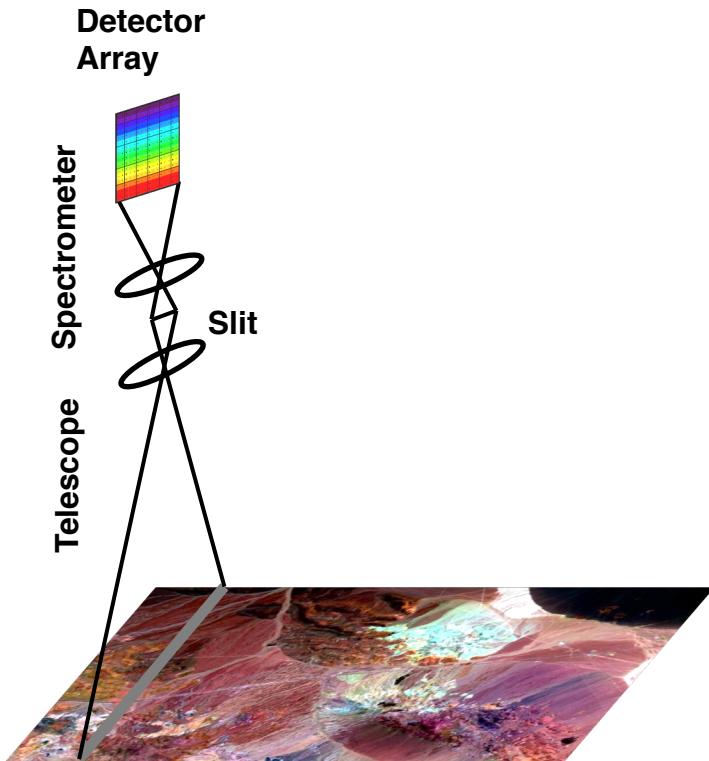
The Averaging Kernel Matrix: retrieval sensitivity to a change in the true state vector

$$\mathbf{A} = \frac{\partial \hat{\mathbf{x}}}{\partial \mathbf{x}} = \mathbf{GK}$$

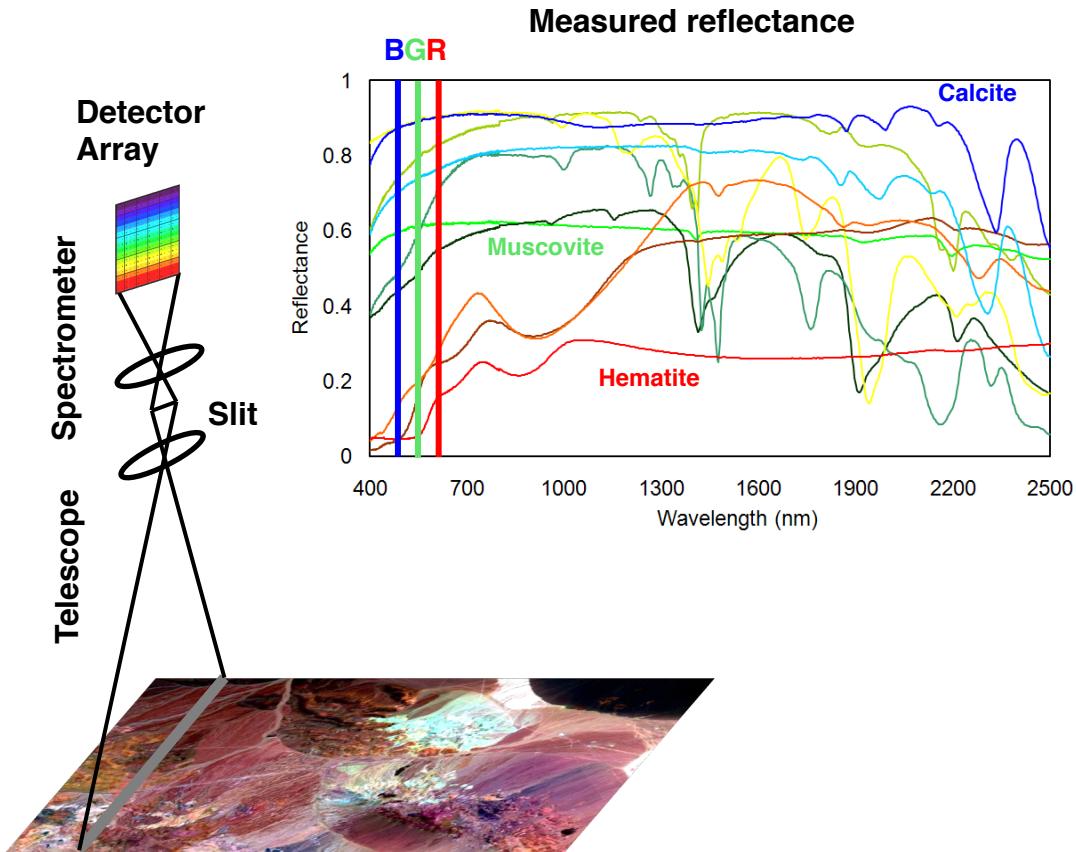
The diagonal shows the *Degrees of Freedom* (DOF) for the retrieved value.



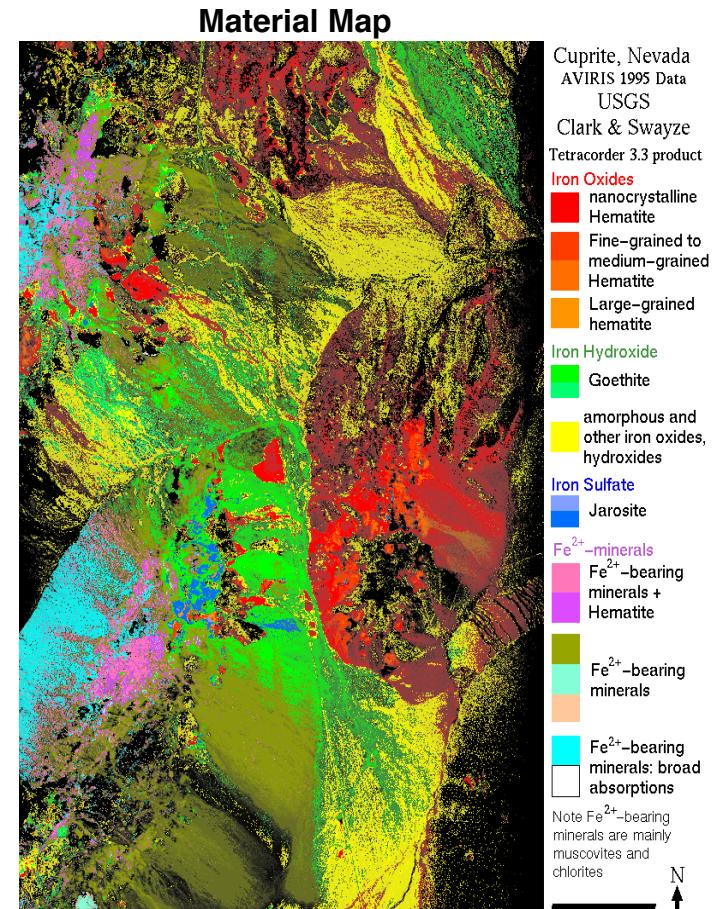
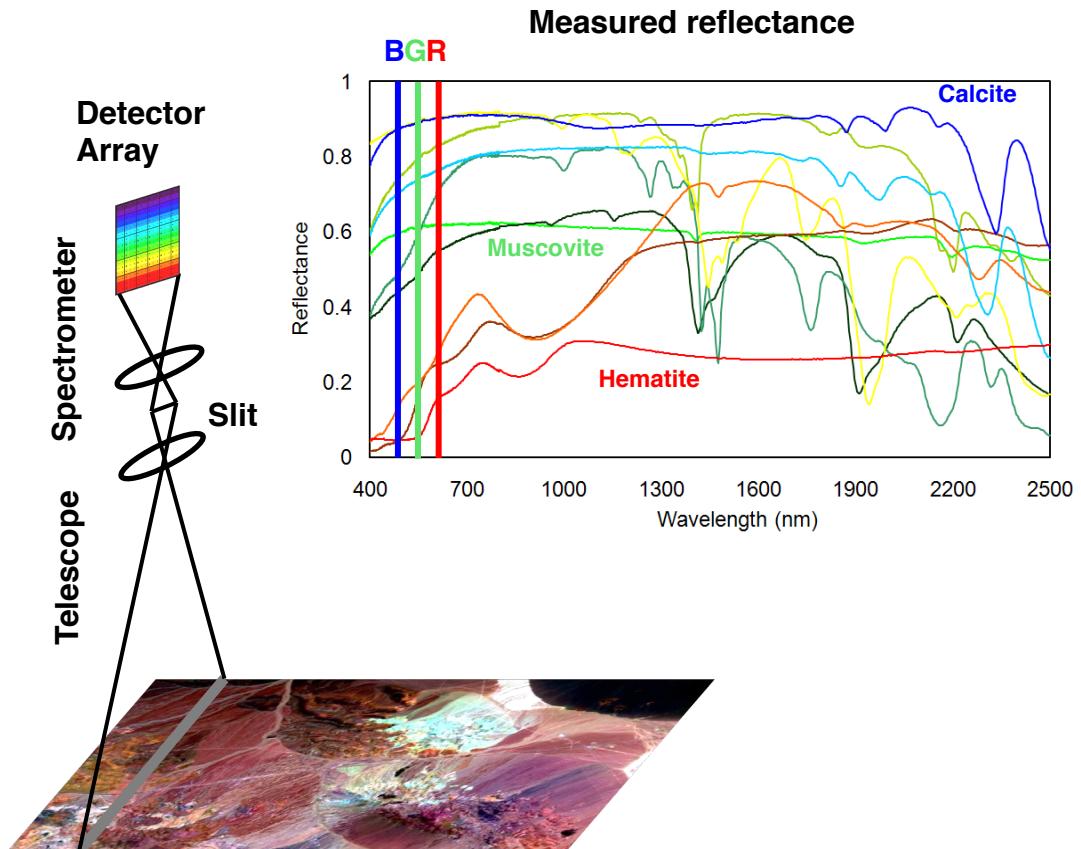
Measurement method



Measurement method



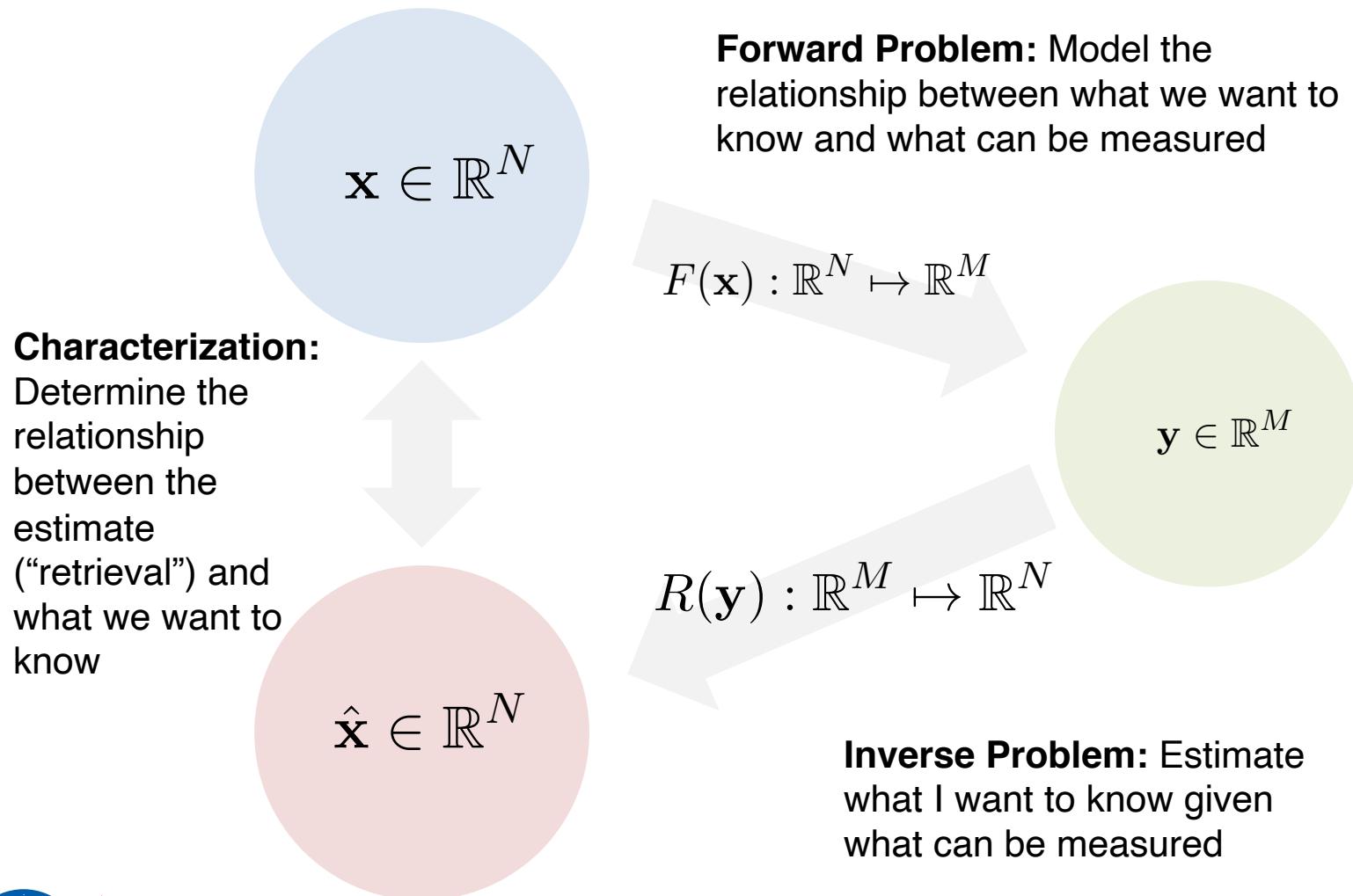
Measurement method



(Courtesy Clark, Swayze)



A tripartite challenge



The Jacobian: The state's influence on an observable

Elements of $F(\mathbf{x})$:

$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \\ \vdots \\ f_M(\mathbf{x}) \end{bmatrix} \quad f_m(\mathbf{x}) : \mathbb{R}^N \rightarrow \mathbb{R}$$

Consider the first order Taylor series expansion:
A local approximation, which is exact for linear problems

$$\mathbf{F}(\mathbf{x} + \delta\mathbf{x}) \approx \mathbf{F}(\mathbf{x}) + \nabla\mathbf{F}(\mathbf{x})\delta\mathbf{x}$$



The Jacobian: The state's influence on an observable

Written explicitly as:

$$\nabla \mathbf{F}(\mathbf{x}) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \dots & \frac{\partial f_1}{\partial x_N} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \dots & \frac{\partial f_2}{\partial x_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_M}{\partial x_1} & \frac{\partial f_M}{\partial x_2} & \dots & \frac{\partial f_M}{\partial x_N} \end{bmatrix} \quad \text{where } x_n = [\mathbf{x}]_n$$

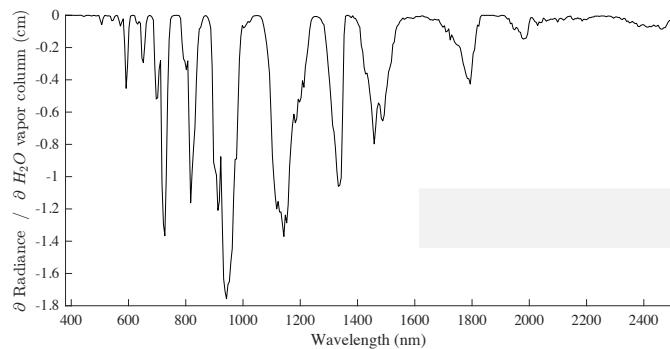
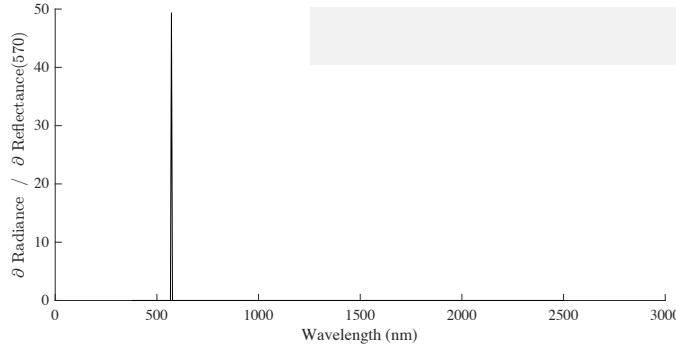
A more compact form:

$$\nabla \mathbf{F}(\mathbf{x}) = \mathbf{K}_x = \mathbf{K}(\mathbf{x})$$



The Jacobian: The state's influence on an observable

A single reflectance value



$$\begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \dots & \frac{\partial f_1}{\partial x_N} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \dots & \frac{\partial f_2}{\partial x_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_M}{\partial x_1} & \frac{\partial f_M}{\partial x_2} & \dots & \frac{\partial f_M}{\partial x_N} \end{bmatrix}$$

Atmospheric H_2O column



From physics to statistics

Given an initial guess \mathbf{x}_0 , how close would the result be it to what we measured?

$$\mathbf{y} - F(\mathbf{x}_0) \approx \mathbf{K}(\mathbf{x} - \mathbf{x}_0) + \boldsymbol{\epsilon}$$

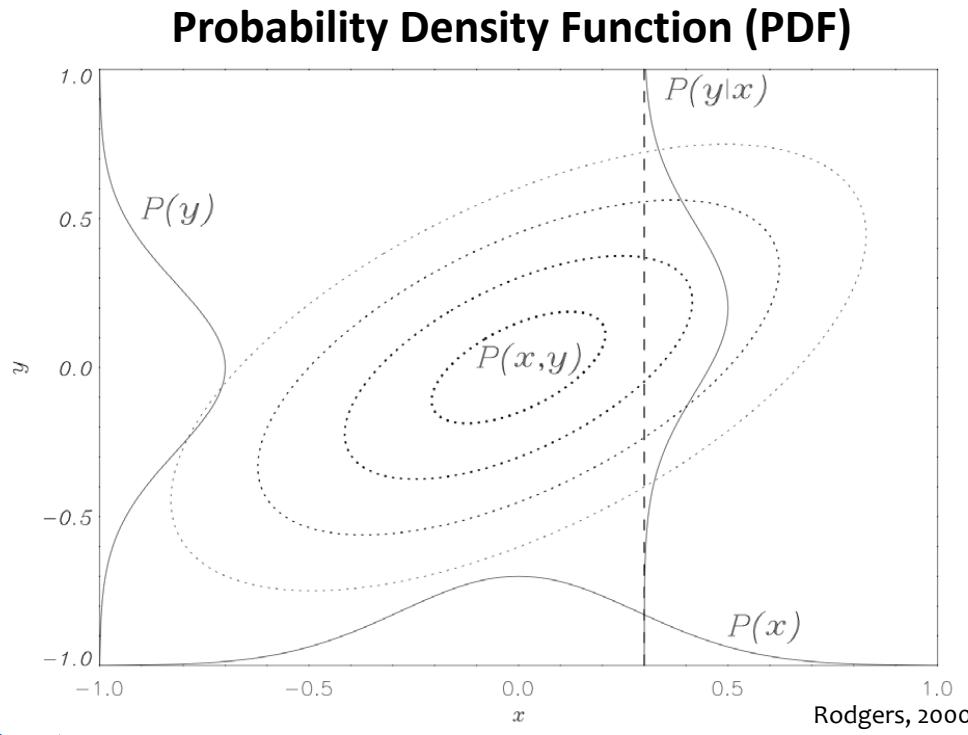
↑
Random perturbation:
Noise and unknowns in
the measurement

In order to say something about the probability of \mathbf{x}_0 we have to know something about the distributions of \mathbf{x} and $\boldsymbol{\epsilon}$



Bayes' theorem

We want to know the probability of \mathbf{x} given \mathbf{y} , i.e. the *conditional distribution* $p(\mathbf{x}|\mathbf{y})$



Conditional distribution

$$p(\mathbf{y}|\mathbf{x}) \triangleq \frac{p(\mathbf{x}, \mathbf{y})}{p(\mathbf{x})}$$

Marginal distribution

$$p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{y}) d\mathbf{y}$$



Bayes' theorem

$$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{p(\mathbf{y})}$$

Conditional probability of measurement given the state vector

Prior probability of state vector

Conditional probability of state vector given a measurement

Marginal probability of measurement (requires integrating over the joint PDF)



Multivariate Gaussian case

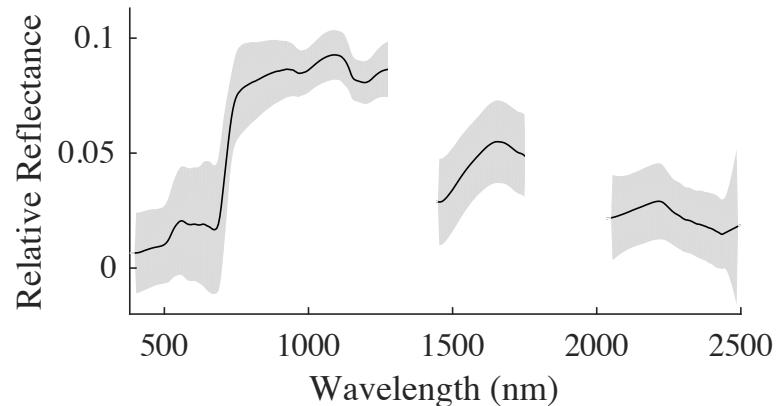
Prior mean and 95% confidence for some vegetation spectra (covariances not shown)

Prior mean

$$E[\mathbf{x}] = \mathbf{x}_a$$

Prior covariance

$$E[(\mathbf{x} - \mathbf{x}_a)(\mathbf{x} - \mathbf{x}_a)^T] = \mathbf{S}_a$$



Prior distribution

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{n/2} |\mathbf{S}_a|^{1/2}} \exp \left[-\frac{1}{2} (\mathbf{x} - \mathbf{x}_a)^T \mathbf{S}_a^{-1} (\mathbf{x} - \mathbf{x}_a) \right]$$



Multivariate Gaussian case

$$E[\mathbf{y} - F(\mathbf{x})] = 0$$

**Observation noise
has zero mean**

$$E[(\mathbf{y} - F(\mathbf{x}))(\mathbf{y} - F(\mathbf{x}))^T] = \mathbf{S}_\epsilon$$

**Observation noise
covariance**

$$p(\mathbf{y}|\mathbf{x}) = \frac{1}{(2\pi)^{m/2} |\mathbf{S}_\epsilon|^{1/2}} \exp \left[-\frac{1}{2} (\mathbf{y} - F(\mathbf{x}))^T \mathbf{S}_\epsilon^{-1} (\mathbf{y} - F(\mathbf{x})) \right]$$

Observation noise distribution

